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L_0-STABLE SPLIT LINEAR MULTISTEP FORMULAS FOR PARABOLIC PDEs

M. J. CASPER and D. A. VOSS
Department of Mathematics, Western Illinois University, Macomb, IL 61455, U.S.A.

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Abstract—New types of split linear multistep methods (SLMMs) are applied to the numerical solution of parabolic differential equations. The formulas derived achieve up to fourth-order in time, and unlike the Crank–Nicolson method, are L_0-stable.

1. INTRODUCTION

In a recent paper Cash [1] investigated two new classes of finite difference schemes for the numerical solution of parabolic partial differential equations. His starting point was to exploit the important fact that all the extrapolation methods considered by Gourlay and Morris [2, 3] for the numerical solution of the constant coefficient, homogeneous equation

$$\frac{\partial u}{\partial t} = Lu, \quad (x, t) \in [0, 1] \times [0 < t \leqslant T], \tag{1}$$

subject to the initial condition

$$u(x, 0) = f(x), \quad x \in [0, 1], \tag{2}$$

and the boundary conditions

$$u(0, t) = u(1, t) = 0, \quad \text{for } t \geqslant 0, \tag{3}$$

can be written as semi-implicit Runge–Kutta methods.

Considering the one-dimensional case defined by $L \equiv \partial^2/\partial x^2$, Cash followed the approach of Gourlay and Morris and replaced L by a suitable finite difference operator. Taking the usual Δx, Δt mesh in x and t, and replacing L in equation (1) by the second-order central difference approximation, gives a system of ordinary differential equations

$$\frac{dy}{dt} = Ay. \tag{4}$$

Here y is an N-vector $((N + 1)\Delta x = 1)$ of unknowns and

$$A = \frac{1}{(\Delta x)^2}\begin{bmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & \bigcirc & \\ & & \ddots & \ddots & \ddots & \\ & \bigcirc & & 1 & -2 & 1 \\ & & & & 1 & -2 \end{bmatrix}$$

has dimension N. Their motivation was to derive L_0-stable (see Definition 1.1) methods which are suitable for solving parabolic equations having high frequency components in the solution. Using Butcher's [4] well-developed theory for Runge–Kutta methods, Cash derived efficient L_0-stable schemes which are at least second-order in time. A particular second-order scheme for equation (4) is given by

$$\begin{aligned}(I + \phi\,\Delta t A)\bar{y}_{n+1} &= (I + (1 - \phi)\,\Delta t A)y_n \\ (I - \phi\,\Delta t A)y_{n+1} &= (I + \tfrac{1}{2}\Delta t A)y_n + (\tfrac{1}{2} - \phi)\,\Delta t A\bar{y}_{n+1}.\end{aligned} \tag{5}$$

The formation of the right-hand sides can be accomplished without any matrix–vector products, and the choice $\phi = 1 - 1/\sqrt{2}$ renders equations (5) L_0-stable while reducing the local truncation error. It is important to observe that both systems of algebraic equations occurring in equations (5) possess the same coefficient matrix, whereas the corresponding second-order formula of Gourlay and Morris [2] utilizes two different coefficient matrices. The formulas derived by Cash [1] apply to the more general parabolic equation

$$\frac{\partial u}{\partial t} = v\frac{\partial^2 u}{\partial x^2} + g(u, u_x), \tag{6}$$

where v is constant and g is a sufficiently smooth function of u and u_x, so that equation (6) with the side conditions (2) and (3) possesses a unique solution. Replacing the partial derivatives u_x and u_{xx} by their second-order central difference approximations transforms equation (6) into a system of ordinary differential equations of the form

$$\frac{dy}{dt} = f(t, y). \tag{7}$$

Formula (5) is an example of a split linear multistep method (SLMM) whose general form [5] when applied to equation (7) is the following.

Predictor.

$$\bar{\alpha}_k \bar{y}_{n+k} - \Delta t\bar{\beta}_k f(t_{n+k}, \bar{y}_{n+k}) = -\sum_{j=0}^{k-1} (\bar{\alpha}_j y_{n+j} - \Delta t\bar{\beta}_j f_{n+j}). \tag{8a}$$

Corrector.

$$\alpha_k y_{n+k} - \Delta t(\beta_k - \theta) f(t_{n+k}, y_{n+k}) = -\sum_{j=0}^{k-1} (\alpha_j y_{n+j} - \Delta t\beta_j f_{n+j}) + \Delta t\theta f(t_{n+k}, \bar{y}_{n+k}), \tag{8b}$$

where $\bar{\beta}_k \neq 0$ and $\beta_k - \theta \neq 0$; that is, both the predictor and corrector are implicit. Applying the SLMM given in equations (8) to the scalar test equation $y' = \lambda y$, $\lambda < 0$, yields the stability equation

$$\sum_{j=0}^{k} [(\alpha_j - q\beta_j)(\bar{\alpha}_k - q\bar{\beta}_k) - \theta q(q\bar{\beta}_j - \bar{\alpha}_j)]r^j = 0, \tag{9}$$

where $q = \lambda\Delta t$.

Definition 1.1

An SLMM given in equations (8) is said to be A_0-stable if the roots $r_i(q)$, $i = 1, \ldots, k$, of equation (9) satisfy $|r_i(q)| < 1$ for $q < 0$; if in addition $\lim_{q\to-\infty} |r_i(q)| = 0$, $i = 1, \ldots, k$, then the formula is said to be L_0-stable.

In Ref. [1], Cash mentioned that it would be of interest to see whether it is possible to obtain an L_0-stable formula of the form (8) with $k = 2$ having order 3 or 4. There, however, he considered a different class of Runge–Kutta formulas, the so-called "look ahead" methods or extended backward differentiation formulas [5, 6]. This produced a third-order one-step scheme involving three systems of algebraic equations utilizing two different coefficient matrices. In another paper [7], Cash further investigated SLMMs based on standard backward differentiation formulas (BDFs). There he derived L-stable formulas suitable for solving stiff initial value problems for ODEs. However, when solving parabolic PDEs by semi-discretization the lesser property of L_0-stability is normally sufficient for the time integrator. This relaxation of the stability requirement allows us to consider split methods based on Adams–Moulton rather than BDF methods. Denoting a k-step SLMM of order p by SLMM(k, p), all the formulas discussed by Cash have $k = p$. Formula (5) belongs to the class SLMM(1, 2), and in Section 2, we reconsider it in that context. In Section 3, we derive efficient, L_0-stable formulas in the classes SLMM(2, 3) and SLMM(3, 4). We also show that there is no corresponding efficient, L_0-stable formula in the class SLMM(2, 4). In Section 4, some numerical results are presented which illustrate the competitive nature of these new formulas when applied to problems possessing high frequency components in their solution.

2. THE CLASS SLMM(1, 2)

The basic idea behind an SLMM is to rewrite the standard linear multistep method

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = \Delta t \sum_{i=0}^{k} \beta_i f_{n+i} \quad (\alpha_k = 1), \tag{10}$$

for system (7) in the form (8b) where the quantity $\bar{y}_{n+k}$ is obtained using the separate implicit predictor (8a). With $\theta \neq 0, \theta \neq \beta_k$ form (8) yields a class of formulas with very good stability properties [7]. It is straightforward to verify that if formula (10) has order p and formula (8a) has order $\geqslant p-1$, then formula (8b) will have order $\geqslant p$. Moreover, to preserve the efficiency of the predictor–corrector pair, the predictor will be specifically constructed as in Ref. [7] so that if formula (8a) is solved for $\bar{y}_{n+k}$ and formula (8b) is solved for y_{n+k}, both using a modified Newton iteration scheme, then the coefficient matrix of both iteration schemes will be

$$I - \phi\, \Delta t \frac{\partial f}{\partial y}, \tag{11}$$

that is, $\phi = \bar{\beta}_k = \beta_k - \theta$. Consequently, for the linear case (4), all the schemes we develop only require one LU decomposition and two forward–backward substitutions per time step.

The class of methods SLMM(1, 2), in efficient mode, has the following form.

Predictor.

$$\bar{y}_{n+1} - y_n = \Delta t[(\tfrac{1}{2} + \theta) f_n + (\tfrac{1}{2} - \theta)\bar{f}_{n+1}]. \tag{12a}$$

Corrector.

$$y_{n+1} - y_n = \Delta t[\tfrac{1}{2} f_n + \theta \bar{f}_{n+1} + (\tfrac{1}{2} - \theta) f_{n+1}]. \tag{12b}$$

From equation (9), their stability polynomial is given by

$$[1 - q(\tfrac{1}{2} - \theta)]^2 r - q^2\theta^2 - (2q + q^2)\theta + \tfrac{1}{4}q^2 - 1 = 0. \tag{13}$$

If $\lambda < 0$ is an estimate of the largest eigenvalue in magnitude of the Jacobian matrix, $\partial f/\partial y$, then using the concept of exponential fitting discussed by Liniger and Willoughby [8], we select θ so that $r = e^q$ is a solution of equation (13). Equation (13) then becomes

$$A(q)\theta^2 + B(q)\theta + C(q) = 0, \tag{14}$$

where

$$A(q) = q^2(e^q - 1), \quad B(q) = (2q - q^2)e^q - (2q + q^2),$$

$$C(q) = \left(1 - q + \frac{q^2}{4}\right)e^q + \left(\frac{q^2}{4} - 1\right).$$

It easily follows that the solutions, $\theta(q)$, of equation (14) satisfy $\lim_{q\to-\infty} \theta(q) = -1/2 \pm 1/\sqrt{2}$, and with $\theta = -1/2 + 1/\sqrt{2}$, method (5) using $\phi = 1 - 1/\sqrt{2}$ is recovered for the linear system $f(t, y) = Ay$.

In the following, we will refer to scheme (12a) and (12b) with the limiting value $\theta = -1/2 + 1/\sqrt{2}$, as method SM12. Of course, if an estimate of a dominant, isolated eigenvalue of $\partial f/\partial y$ can be found cheaply, we can use exponential fitting throughout the range of integration. From equation (14) using

$$\theta(q) = (-B(q) - \sqrt{B^2(q) - 4A(q)C(q)})/2A(q), \tag{15}$$

we will refer to the corresponding fitted method (12a) and (12b) as SM12E. Table 1 illustrates that $\theta(q)$ is a slowly varying function and remains reasonably close to its limiting value $\theta = -1/2 + 1/\sqrt{2} \approx 0.2071$ even for values of q close to zero.

The local truncation error (LTE) for these methods has the form

$$\theta^2(\Delta t)^3 \frac{\partial f}{\partial y} y_n'' - \tfrac{1}{12}(\Delta t)^3 y_n''' + O((\Delta t)^4). \tag{16}$$

Table 1. Parameter value from exponential fitting

q	$\theta(q)$
-5.0	0.2502
-10.0	0.2325
-50.0	0.2128
-100.0	0.2100
-500.0	0.2077
-1000.0	0.2074
$-\infty$	0.2071

Consequently, since $\theta(q) > 1$ for $q > -1.34$, SM12E will possess a relatively larger LTE than SM12 for values of q near zero. However, for problems where exponential fitting is of interest, the fitting parameter q is often much smaller than -5. In the next section exponential fitting is used to construct higher-order SLMMs which are strongly damped at infinity.

3. HIGHER-ORDER METHODS

First, we investigate the class SLMM(2, 3) based on splitting the two-step, third-order Adams–Moulton method

$$y_{n+2} - y_{n+1} = \Delta t\left(-\tfrac{1}{12}f_n + \tfrac{2}{3}f_{n+1} + \tfrac{5}{12}f_{n+2}\right). \tag{17}$$

For the predictor, we select a second-order, two parameter family [9]

$$\bar{y}_{n+2} - (1+b)y_{n+1} + by_n = \Delta t\left\{cf_n + \left(\tfrac{1}{2}(1-3b) - 2c\right)f_{n+1} + \left(\tfrac{1}{2}(1+b) + c\right)\bar{f}_{n+2}\right\}. \tag{18}$$

From equation (8b) it follows that the splitting of the corrector will be such that the coefficient of f_{n+2} is $(\frac{5}{12} - \theta)$. Therefore, in order for the predictor–corrector pair to be in efficient mode we require

$$\tfrac{1}{2}(1+b) + c = \tfrac{5}{12} - \theta$$

or

$$c = -\frac{1}{12} - \frac{b}{2} - \theta.$$

This choice of c leads to an SLMM(2, 3) of the form

Predictor.

$$\bar{y}_{n+2} - (1+b)y_{n+1} + by_n = \Delta t\left\{\left(-\frac{1}{12} - \frac{b}{2} - \theta\right)f_n + \left(\frac{2}{3} - \frac{b}{2} + 2\theta\right)f_{n+1} + \left(\frac{5}{12} - \theta\right)\bar{f}_{n+2}\right\}. \tag{19a}$$

Corrector.

$$y_{n+2} - y_{n+1} = \Delta t\left\{-\frac{1}{12}f_n + \frac{2}{3}f_{n+1} + \theta\bar{f}_{n+2} + \left(\frac{5}{12} - \theta\right)f_{n+2}\right\}, \tag{19b}$$

where the parameters b and θ are yet to be determined. The stability equation for method (19a) and (19b) has the form

$$\pi(r, q) \equiv C_2r^2 + C_1r + C_0 = 0, \tag{20}$$

where the coefficients are in terms of b, θ and q. Following the exponential fitting approach of Liniger and Willoughby [8], we force $r_1 = e^q$ and $r_2 = 0$ to be roots of equation (20) where, as in Section 2, $q = \lambda\,\Delta t$ and $\lambda < 0$ is an estimate of the largest eigenvalue in magnitude of $\partial f/\partial y$. Thus

$$b = \frac{-\dfrac{1}{12} + \left(\dfrac{5}{144} - \dfrac{\theta}{6} - \theta^2\right)q}{\theta(1 + q/2)}, \tag{21a}$$

and θ satisfies the quadratic equation

$$\tilde{A}(q)\theta^2 + \tilde{B}(q)\theta + \tilde{C}(q) = 0, \tag{21b}$$

where, with $\tilde{D} = (q-2)(q+2)$,

$$\tilde{A}(q) = q^2(e^q - 2 - \tilde{D}),$$

$$\tilde{B}(q) = (2q - \tfrac{5}{6}q^2)e^q - 2q - \tfrac{4}{3}q^2 - \tfrac{1}{6}q^2\tilde{D},$$

$$\tilde{C}(q) = (1 - \tfrac{5}{6}q + \tfrac{25}{144}q^2)e^q - 1 - \tfrac{1}{4}q + \tfrac{5}{18}q^2 - \tfrac{1}{12}q\tilde{D} + \tfrac{5}{144}q^2\tilde{D}.$$

It can be shown that θ and b have limits at $-\infty$ given by

$$\lim_{q\to-\infty} \theta = -\frac{1}{4} \pm \frac{\sqrt{6}}{6},$$

$$\lim_{q\to-\infty} b = \frac{5}{72\theta} - 2\theta - \frac{1}{3}.$$

The choice

$$\theta = -\frac{1}{4} + \frac{\sqrt{6}}{6} \approx 0.1582, \qquad b = \frac{5}{72\theta} - 2\theta - \frac{1}{3} \approx -0.2110 \tag{22}$$

minimizes the coefficient of the first term in the LTE of the predictor–corrector pair (19a) and (19b) which has the form

$$\theta\left(\frac{b}{12} + \theta\right)(\Delta t)^4 \frac{\partial f}{\partial y} y_n''' - \frac{1}{24}(\Delta t)^4 y_n'''' + 0((\Delta t)^5). \tag{23}$$

The method (19a) and (19b) corresponding to the limiting values of the parameters (22) will be denoted by SM23.

Theorem 3.1

SM23 is L_0-stable.

Proof. By construction the roots $r_1(q)$ and $r_2(q)$ of the stability polynomial $\pi(r, q)$ in equation (20) satisfy

$$\lim_{q\to-\infty} |r_i(q)| = 0, \quad i = 1, 2.$$

Therefore, we need to show that $|r_i(q)| < 1$ for all $q < 0$; that is, $\pi(r, q)$ is a Schur polynomial [9] for $q < 0$. Defining the polynomials

$$\hat{\pi}(r, q) = C_0 r^2 + C_1 r + C_2$$

and

$$\pi_1(r, q) = \frac{1}{r}[\hat{\pi}(0, q)\pi(r, q) - \pi(0, q)\hat{\pi}(r, q)],$$

then by a theorem of Schur [10], $\pi(r, q)$ is a Schur polynomial for $q < 0$ if, and only if,

$$|\hat{\pi}(0, q)| > |\pi(0, q)| \tag{24a}$$

and

$$\pi_1(r, q) \text{ is a Schur polynomial.} \tag{24b}$$

With b and θ from equation (22) we find that

$$C_0 = \tfrac{1}{9}(-2 + \sqrt{6})q,$$

$$C_1 = -1 - \tfrac{1}{9}(-5 + 4\sqrt{6})q,$$

$$C_2 = [1 - \tfrac{1}{6}(4 - \sqrt{6})q]^2.$$

Inequality (24a) is true if $|C_2| > |C_0|$ for $q < 0$, or

$$S(q) \equiv \tfrac{1}{36}(4-\sqrt{6})^2 q^2 + \tfrac{2}{9}(-7+2\sqrt{6})q + 1 > 0,$$

for $q < 0$. $S(q)$ has an absolute minimum at $q^* = 4(7-2\sqrt{6})/(4-\sqrt{6})^2$, and since $S(q^*) > 0$, inequality (24a) follows. The polynomial $\pi_1(r, q)$ has the single root

$$r(q) = \frac{1 + \frac{1}{9}(-5+4\sqrt{6})q}{[1-\frac{1}{6}(4-\sqrt{6})q]^2 + \frac{1}{9}(-2+\sqrt{6})q},$$

from which it follows that $r(0) = 1$ and $\lim_{q \to -\infty} r(q) = 0$. Moreover, with

$$q^{**} = \{9[11 - 4\sqrt{6} + \sqrt{-85+40\sqrt{6}}]\}/(151 - 64\sqrt{6}) \approx -7.5,$$

$r(q)$ is decreasing on $(-\infty, q^{**})$ and increasing on $(q^{**}, 0)$. Since $r(q^{**}) \approx -0.36$, $\pi_1(r, q)$ is a Schur polynomial for $q < 0$ and the theorem follows.

Analogous to SM12E, we denote the exponentially fitted method (19a) and (19b) by SM23E where $b(q)$ is given in equation (21a) and $\theta(q)$ is a solution of equation (21b), namely

$$\theta(q) = (-\tilde{B}(q) - \sqrt{\tilde{B}^2(q) - 4\tilde{A}(q)\tilde{C}(q)})/2\tilde{A}(q). \tag{25}$$

Similarly, Table 2 illustrates that $\theta(q)$ and $b(q)$ are slowly varying functions and remain reasonably close to their limiting values, given in equation (22), even for values of q relatively close to zero. We note that $b(q)$ is undefined for $q = -2$, and that $b(q)$ and $\theta(q)$ switch signs for $-2 < q < 0$. However, as mentioned in the previous section, the fitting parameter q is normally smaller than -5 and could artificially be set to -5 in these instances.

For the linear system (4), our basic predictor–corrector scheme (19a) and (19b) has the form

$$(I - \bar{\beta}_2 \Delta t A)\bar{y}_{n+2} = \left[-bI + \Delta t\left(-\frac{1}{12} - \frac{b}{2} - \theta\right)A\right]y_n + \left[(1+b)I + \Delta t\left(\frac{2}{3} - \frac{b}{2} + 2\theta\right)A\right]y_{n+1}, \tag{26a}$$

$$(I - \bar{\beta}_2 \Delta t A)y_{n+2} = -\frac{1}{12}\Delta t A y_n + \left[I + \frac{2}{3}\Delta t A\right]y_{n+1} + \theta A \bar{y}_{n+2}, \tag{26b}$$

where $\bar{\beta}_2 = \frac{5}{12} - \theta$. The complete algorithm then consists of solving equation (26a) for $\bar{y}_{n+2}$ and equation (26b) for y_{n+2}. We now show that this can be accomplished without forming any matrix products on the right-hand side of equations (26a) and (26b) in a manner similar to that of Cash [1] for scheme (5). Considering equation (26b), we solve equations of the form

$$(I - \bar{\beta}_2 \Delta t A)y^{(0)}_{n+2} = m_1 \bar{\beta}_2 y_n + m_2 \bar{\beta}_2 y_{n+1} + m_3 \bar{\beta}_2 \bar{y}_{n+2}, \tag{27a}$$

$$y_{n+2} = m_4 y_n + m_5 y_{n+1} + m_6 \bar{y}_{n+2} + y^{(0)}_{n+2}\bar{\beta}_2, \tag{27b}$$

where the m_i, $i = 1, \ldots, 6$, are to be determined. Then from equation (27b) we have

$$(I - \bar{\beta}_2 \Delta t A)y_{n+2} = m_4(I - \bar{\beta}_2 \Delta t A)y_n + m_5(I - \bar{\beta}_2 \Delta t A)y_{n+1} + m_6(I - \bar{\beta} \Delta t A)\bar{y}_{n+2} + m_1 y_n + m_2 y_{n+1} + m_3 \bar{y}_{n+2}.$$

Using equation (26b) we now require

$$(m_1 + m_4)I - m_4 \bar{\beta}_2 \Delta t A = -\tfrac{1}{12}\Delta t A,$$

$$(m_2 + m_5)I - m_5 \bar{\beta}_2 \Delta t A = I + \tfrac{2}{3}\Delta t A,$$

$$(m_3 + m_6)I - m_6 \bar{\beta}_2 \Delta t A = \theta A,$$

so that

$$m_1 = -\frac{1}{12\bar{\beta}_2}, \quad m_2 = 1 + \frac{2}{3\bar{\beta}_2}, \quad m_3 = \frac{\theta}{\bar{\beta}_2}, \quad m_4 = \frac{1}{12\bar{\beta}_2}, \quad m_5 = -\frac{2}{3\bar{\beta}_2}, \quad m_6 = -\frac{\theta}{\bar{\beta}_2}.$$

Table 2 Parameter values from exponential fitting

q	$\theta(q)$	$b(q)$
−5.0	0.1904	−0.2907
−10.0	0.1781	−0.2575
−50.0	0.1629	−0.2210
−100.0	0.1608	−0.2166
−500.0	0.1588	−2.2123
−1000.0	0.1585	−0.2115
$-\infty$	0.1582	−0.2110

The result is that equation (26b) is replaced by

$$(I - \bar{\beta}_2 \Delta t A) y_{n+2}^{(0)} = -\tfrac{1}{12} y_n + (\bar{\beta}_2 + \tfrac{2}{3}) y_{n+1} + \theta \bar{y}_{n+2}, \tag{28a}$$

$$y_{n+2} = (\tfrac{1}{12} y_n - \tfrac{2}{3} y_{n+1} - \theta \bar{y}_{n+2} + y_{n+2}^{(0)})\, \bar{\beta}_2. \tag{28b}$$

A similar analysis reveals that equation (26a) is replaced by

$$(I - \bar{\beta}_2 \Delta t A) \bar{y}_{n+2}^{(0)} = -\left[b\left(\bar{\beta}_2 + \frac{1}{2}\right) + \frac{1}{12} + \theta \right] y_n + \left[\bar{\beta}_2 (1 + b) + \frac{2}{3} - \frac{b}{2} + 2\theta \right] y_{n+1}, \tag{29a}$$

$$\bar{y}_{n+2} = \left[\left(\frac{1}{12} + \frac{b}{2} + \theta \right) y_n - \left(\frac{2}{3} - \frac{b}{2} + 2\theta \right) y_{n+1} + \bar{y}_{n+2}^{(0)} \right] / \bar{\beta}_2. \tag{29b}$$

We note that our algorithms can be applied to nonlinear parabolic PDEs in a straightforward fashion. As mentioned by Cash [1], the two most straightforward ways are to use a modified Newton method, which for the predictor (19a) has the form

$$\begin{aligned}(I - \bar{\beta}_2 \Delta t J)(\bar{y}_{n+2}^{(p+1)} - \bar{y}_{n+2}^{(p)}) = -\bar{y}_{n+2}^{(p)} + (1 + b) y_{n+1} - b y_n + \Delta t \Bigg[\left(-\frac{1}{12} - \frac{b}{2} - \theta \right) f(t_n, y_n) \\ + \left(\frac{2}{3} - \frac{b}{2} + 2\theta \right) f(t_{n+1}, y_{n+1}) + \left(\frac{5}{12} - \theta \right) f(t_{n+2}, \bar{y}_{n+2}^{(p)}) \Bigg],\end{aligned}$$

$$J \approx \frac{\partial f}{\partial y}(t_{n+2}, \bar{y}_{n+2}^{(p)}), \tag{30}$$

or to use quasi-linearization. In the latter approach an initial estimate $\bar{y}_{n+2}^{(0)}$ is made to $\bar{y}_{n+2}$, and then the linear system

$$\frac{\mathrm{d}\Delta y}{\mathrm{d}y} = \frac{\partial f}{\partial y}(t_{n+2}, \bar{y}_{n+2}^{(0)})\, \Delta y \tag{31}$$

is solved for Δy yielding $\bar{y}_{n+2}^{(0)} + \Delta y$ as our next approximation to $\bar{y}_{n+2}$ for continuing the iterative process. As in Cash's algorithms, since equation (31) has the same form as equation (4) with A replaced by the Jacobian matrix $\partial f / \partial y$, the same procedure described in equations (28a) and (28b), (29a) and (29b) can be used to solve equation (31).

Lastly, in this section, we consider fourth-order SLMMs. We first show that there is no L_0-stable method in the class SLMM(2, 4) that preserves the efficiency described in form (11), namely, $\bar{\beta}_2 = \beta_2 - \theta$. To achieve fourth-order we need to split the Milne–Simpson method

$$y_{n+2} - y_n = \Delta t \{ \tfrac{1}{3} f_n + \tfrac{4}{3} f_{n+1} + \tfrac{1}{3} f_{n+2} \}. \tag{32}$$

The two-step predictor must be at least third-order and, consequently, in efficient mode we obtain the SLMM

Predictor.

$$\bar{y}_{n+2} + 12\theta y_{n+1} - (1 + 12\theta) y_n = \Delta t \{ (\tfrac{1}{3} + 5\theta) f_n + (\tfrac{4}{3} + 8\theta) f_{n+1} + (\tfrac{1}{3} - \theta) \bar{f}_{n+2} \}. \tag{33a}$$

Corrector.

$$y_{n+2} - y_n = \Delta t \{ \tfrac{1}{3} f_n + \tfrac{4}{3} f_{n+1} + \theta \bar{f}_{n+2} + (\tfrac{1}{3} - \theta) f_{n+2} \}. \tag{33b}$$

From equation (9), the stability equation is

$$C_2 r^2 + C_1 r + C_0 = 0, \tag{34}$$

where

$$C_0 = -1 - (2\theta + 12\theta^2)q + (\tfrac{1}{4} - \tfrac{2}{3}\theta - 5\theta^2)q^2,$$

$$C_1 = -(\tfrac{4}{3} - 12\theta^2)q + (\tfrac{3}{4} - \tfrac{2}{3}\theta - 8\theta^2)q^2,$$

$$C_2 = (1 - (\tfrac{1}{3} - \theta)q)^2.$$

As $q \to -\infty$, equation (34) has real roots given by

$$r_{1,2}(\theta) = \frac{-2(1 - 6\theta - 18\theta^2) \pm \sqrt{4(1 - 6\theta - 18\theta^2)^2 - (1 - 3\theta)^2(1 - 6\theta - 45\theta^2)}}{(1 - 3\theta)^2},$$

and there is no value of θ which makes both of these zero.

Finally, we show that there do exist L_0-stable methods in the class SLMM(3, 4) generated by splitting the three-step, fourth-order Adams–Moulton method

$$y_{n+3} - y_{n+2} = \frac{\Delta t}{24}(f_n - 5f_{n+1} + 19f_{n+2} + 9f_{n+3}). \tag{35}$$

In efficient mode, this leads to the following predictor–corrector pair.

Predictor.

$$y_{n+3} - (1 + a + b)y_{n+2} + ay_{n+1} + by_n = \Delta t\left\{\left(\frac{1}{24} - \frac{b}{3} + \frac{a}{12} + \theta\right)f_n\right.$$
$$\left. + \left(-\frac{5}{24} - \frac{4}{3}b - \frac{2}{3}a - 3\theta\right)f_{n+1} + \left(\frac{19}{24} - \frac{b}{3} - \frac{5}{12}a + 3\theta\right)f_{n+2} + \left(\frac{9}{24} - \theta\right)\bar{f}_{n+3}\right\}. \tag{36a}$$

Corrector.

$$y_{n+3} - y_{n+2} = \Delta t\{\tfrac{1}{24}f_n - \tfrac{5}{24}f_{n+1} + \tfrac{19}{24}f_{n+2} + \theta\bar{f}_{n+3} + (\tfrac{9}{24} - \theta)f_{n+3}\}. \tag{36b}$$

The stability equation for scheme (36a) and (36b) will be a cubic polynomial with coefficients depending on the parameters a, b and θ. Utilizing exponential fitting, we force $r_1 = e^q$ and $r_2 = r_3 = 0$ to be roots of the stability equation yielding

$$a = \frac{-\frac{5}{24} + (-\frac{3}{64} - \frac{5}{12}\theta - 3\theta^2)q + (\frac{1}{64} - \frac{1}{4}\theta - \frac{1}{3}\theta^2)q^2}{\theta(1 + q + \frac{1}{3}q^2)}, \tag{37}$$

$$b = \frac{\frac{1}{24} + (-\frac{1}{192} + \frac{1}{12}\theta + \theta^2)q + (-\frac{1}{256} + \frac{1}{48}\theta + \frac{5}{12}\theta^2)q^2}{\theta(1 + q + \frac{1}{3}q^2)}, \tag{38}$$

and θ satisfies the quadratic equation

$$\hat{A}(q)\theta^2 + \hat{B}(q)\theta + \hat{C}(q) = 0 \tag{39}$$

where, with $\hat{D} = 1/(1 + q + \frac{1}{3}q^2)$,

$$\hat{A}(q) = q^2e^q - 3q^2 + q^2(2 + q - \tfrac{1}{6}q^2)\hat{D}$$

$$\hat{B}(q) = (2q - \tfrac{3}{4}q^2)e^q - 2q - \tfrac{19}{12}q^2 + q^2(\tfrac{1}{3} + \tfrac{1}{12}q - \tfrac{7}{72}q^2)\hat{D}$$

$$\hat{C}(q) = (1 - \tfrac{3}{4}q + \tfrac{9}{64}q^2)e^q - 1 - \tfrac{5}{12}q + \tfrac{19}{64}q^2 + q(\tfrac{1}{6} - \tfrac{1}{48}q - \tfrac{37}{576}q^2 + \tfrac{7}{384}q^3)\hat{D}.$$

It follows that θ, a, and b have limits at $-\infty$ given by

$$\lim_{q\to-\infty}\theta = -\frac{15}{88} \pm \frac{3}{22}\sqrt{5},$$

$$\lim_{q\to-\infty} a = \frac{9}{64\theta} - 7\theta - \frac{3}{4},$$

$$\lim_{q\to-\infty} b = -\frac{3}{256\theta} - \frac{5}{4}\theta + \frac{1}{16}.$$

The choice

$$\theta = -\frac{15}{88} + \frac{3}{22}\sqrt{5} \approx 0.1345, \quad a \approx -0.6454, \quad b \approx 0.1434, \tag{40}$$

minimizes the coefficient of the first term in the LTE of predictor–corrector pair (36a) and (36b) which has the form

$$\theta\left(\frac{a}{24} + \theta\right)(\Delta t)^5 \frac{\partial f}{\partial y} y_n^{iv} - \frac{19}{720}(\Delta t)^5 y_n^{v} + 0((\Delta t)^6). \tag{41}$$

An analysis similar to that in Theorem 3.1 establishes that method (36a) and (36b) with the limiting values of the parameters (40) is L_0-stable, and the corresponding method will be denoted SM34. As with previous fitted methods, we denote by SM34E the method corresponding to the choice

$$\theta(q) = (-\hat{B}(q) - \sqrt{\hat{B}^2(q) - 4\hat{A}(q)\hat{C}(q)})/2\hat{A}(q), \tag{42}$$

where $a(q)$ and $b(q)$ are given in equations (37) and (38). Like the lower-order SLMMs, when applied to the linear system (4), the new fourth-order schemes involve the solution of two linear systems possessing the same coefficient matrix; in addition, the right-hand side of these equations can be formed without any matrix products.

4. NUMERICAL RESULTS

We expect the L_0-stable SLMMs derived in the previous sections to be particularly useful for solving parabolic equations having high frequency components in the solution. Cash [1] identifies the following three classes of problems whose solutions typically exhibit such behavior:

(a) problems where the boundary conditions are discontinuous;
(b) problems where the solution decays very rapidly;
(c) "stiff" parabolic equations.

In this section we present the numerical results obtained for Cash's [1] examples of each of these three classes of problems. For comparative purposes, we also include the second-, third- and fourth-order split BDF methods presented by Cash [7], and belonging to class SLMM(2, 2), SLMM(3, 3) and SLMM(4, 4), respectively. We denote the first by SM22, which is the standard BDF given by

$$y_{n+2} - \tfrac{4}{3}y_{n+1} + \tfrac{1}{3}y_n = \tfrac{2}{3}\Delta t f_{n+2}. \tag{43}$$

The second, denoted by SM33, has the form

Predictor.

$$\bar{y}_{n+3} - (\tfrac{18}{11} + \tfrac{5}{2}\theta)y_{n+2} + (\tfrac{9}{11} + 4\theta)y_{n+1} - (\tfrac{2}{11} + \tfrac{3}{2}\theta)y_n = (\tfrac{6}{11} - \theta)\Delta t\bar{f}_{n+3}. \tag{44}$$

Corrector.

$$y_{n+3} - \tfrac{18}{11}y_{n+2} + \tfrac{9}{11}y_{n+1} - \tfrac{2}{11}y_n = \Delta t[(\tfrac{6}{11} - \theta)f_{n+3} + \theta\bar{f}_{n+3}], \tag{45}$$

and the third, denoted SM44, is defined as follows:

Predictor.

$$\bar{y}_{n+4} - (\tfrac{48}{25} + \tfrac{13}{3}\theta)y_{n+3} + (\tfrac{36}{25} + \tfrac{19}{2}\theta)y_{n+2} - (\tfrac{16}{25} + 7\theta)y_{n+1} + (\tfrac{3}{25} + \tfrac{11}{6}\theta)y_n = (\tfrac{12}{25} - \theta)\Delta t\bar{f}_{n+4}. \quad (46)$$

Corrector.

$$y_{n+4} - \tfrac{48}{25}y_{n+3} + \tfrac{36}{25}y_{n+2} - \tfrac{16}{25}y_{n+1} + \tfrac{3}{25}y_n = \Delta t[(\tfrac{12}{25} - \theta)f_{n+4} + \theta\bar{f}_{n+4}]. \quad (47)$$

Cash listed these, and higher-order formulas, for solving stiff systems of ODEs where the stability requested is more severe than L_0-stability. In particular, SM22 is L-stable, SM33 is L-stable for $\theta \in (-0.29, -0.1)$, and SM44 is $L(\alpha)$-stable with $\alpha > 89.990°$ for $\theta = -0.36$. We select values for θ so that SM33 and SM44 are exponentially fitted at $-\infty$; an analysis, similar to that in the previous section, yields $\theta = -2(2 \pm \sqrt{22})/33$ and $\theta = 6(-3 \pm 5\sqrt{3})/275$, respectively. Using the Routh–Hurwitz criterion [9] it follows that SM33 and SM44 are L_0-stable for both corresponding θ values. In the following examples we use $\theta = -2(2 - \sqrt{22})/33 \approx 0.163$ which minimizes the coefficient of the first term in the LTE of SM33

$$\tfrac{11}{6}\theta^2(\Delta t)^4\frac{\partial f}{\partial y}y''' - \tfrac{3}{22}(\Delta t)^4 y_n^{iv} + O((\Delta t)^5), \quad (48)$$

and $\theta = -6(3 - 5\sqrt{3})/275 \approx 0.123$ which minimizes the coefficient of the first term in the LTE of SM44

$$\tfrac{25}{12}\theta^2(\Delta t)^5\frac{\partial f}{\partial y}y^{iv} - \tfrac{12}{125}(\Delta t)^5 y_n^{v} + O((\Delta t)^6). \quad (49)$$

Example 1

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad u(0,t) = u(2,t) = 0, \quad u(x,0) = 1.$$

True solution.

$$u(x,t) = \sum_{n=1}^{\infty}[1 - (-1)^n]\frac{2}{n\pi}\sin\left(\frac{n\pi x}{2}\right)\exp\left(\frac{-n^2\pi^2 t}{4}\right).$$

It is well-known that methods which are A-stable but not L_0-stable, such as the Crank–Nicolson method, experience difficulty with this problem due to undamped oscillatory components of the solution. In Table 3, we give the maximum errors obtained using methods in SLMM(k,p), where $p = 2$ or 3. In all of our examples, the true solution was used to provide any missing starting values.

From Table 3, we note that all four methods perform well even for large values of $r = \Delta t/(\Delta x)^2$. We also observe that the split BDF methods, SM22 and SM33, require an additional starting value and are less accurate with these meshsizes than SM12 and SM23, respectively. This is probably because the latter two methods have smaller error constants in their LTE [see expressions (16) and (23)].

Table 3. Maximum error at $t = 1.2$

Δx	Δt	SM12	SM22	SM23	SM33
0.05	0.2	0.19E − 2	0.18E − 1	0.83E − 3	0.46E − 2
0.05	0.1	0.43E − 3	0.41E − 2	0.15E − 3	0.56E − 3
0.025	0.05	0.10E − 3	0.99E − 3	0.31E − 4	0.80E − 4

Example 2

$$\frac{\partial u}{\partial t} = v\frac{\partial^2 u}{\partial x^2}, \quad u(0,t) = u(1,t) = 0, \quad u(x,0) = \sin \pi x.$$

True solution. $u(x,t) = \exp(-\pi^2 vt)\sin \pi x$.

Schemes which are A-stable but not L_0-stable can experience difficulties with problems of this type due to their inability to correctly follow the rapidly decaying solution in time. In Tables 4 and 5 we give the results obtained for the integration of the above problem using the third- and fourth-order SLMMs, respectively.

The eigenvalues of the matrix A occurring in equation (4) are

$$\sigma_i = \frac{-4}{(\Delta x)^2}\sin^2\left(\frac{i\pi}{2(N+1)}\right), \quad i = 1, \ldots, N,$$

and, consequently, those of the corresponding matrix for the above problem are $\lambda_i = v\sigma_i$, $i = 1, \ldots, N$. The free parameters occurring in the descriptions of SM23E and SM34E were determined by fitting at $q = \Delta t\lambda_N$. With $v = 1$, SM23 was consistently more accurate than either SM23E or SM33. In addition, with $v = 1$, SM34 and SM34E perform about the same on this problem and are more accurate than SM44 using the larger time steps. However, as v is increased, SM23E and SM33 were able to follow the rapidly decaying solution more closely for the larger time step. While all three third-order methods are L_0-stable, the parasitic solution associated with SM23E is damped out exactly, while those of SM33 decrease more rapidly than that of SM33 in this case. As the mesh is refined, the SLMMs generated by Adams formulas perform better than those generated by BDFs with the fourth-order formulas yielding increased accuracy.

Table 4. Maximum error at $t = 1$

Δx	Δt	t	SM23	SM23E	SM33
0.1	0.1	1.0	0.19E − 4	0.68E − 4	0.15E − 3
0.05	0.05	1.0	0.24E − 5	0.13E − 4	0.17E − 4
0.025	0.025	1.0	0.42E − 6	0.19E − 5	0.18E − 5
0.1	0.1	5.0	0.38E − 4	0.32E − 6	0.36E − 5
0.05	0.05	5.0	0.16E − 11	0.35E − 10	0.70E − 8
0.025	0.025	5.0	0.45E − 20	0.25E − 20	0.32E − 14

Table 5. Maximum error at $t = 1$

Δx	Δt	t	SM34	SM34E	SM44
0.1	0.1	1.0	0.81E − 5	0.69E − 5	0.29E − 3
0.05	0.05	1.0	0.48E − 6	0.47E − 6	0.69E − 5
0.025	0.025	1.0	0.22E − 6	0.22E − 6	0.11E − 6
0.1	0.1	5.0	0.90E − 3	0.74E − 3	0.64E − 4
0.05	0.05	5.0	0.88E − 7	0.77E − 7	0.59E − 6
0.025	0.025	5.0	0.35E − 21	0.28E − 21	0.14E − 10

Example 3

$$\frac{\partial u}{\partial t} = v\frac{\partial^2 u}{\partial x^2}, \quad u(0, t) = u(1, t) = 0, \quad u(x, 0) = \sin \pi x + \sin k\pi x, \quad k \gg 1.$$

True solution. $u(x, t) = \exp(-\pi^2 vt)\sin \pi x + \exp(-k^2\pi^2 vt)\sin k\pi x$.

As k increases, equations of this type have characteristics similar to model stiff equations. Cash [1] notes that A-stable methods, although giving a stable representation for the rapidly decreasing solution $\exp(-k^2\pi^2 vt)\sin k\pi x$, will not damp it sufficiently rapidly but will instead represent it as oscillating solution which soon swamps the required solution. With $\Delta x = \Delta t = 0.05$, Table 6 contains the results of all nine SLMMs being considered and the Crank–Nicolson, denoted CN, for $v = 1$ and a range of values of k.

It can be seen from Table 6 that all SLMMs follow the solution correctly, with SM34 being the most accurate at $t = 2$ for all values of k; in addition, note the Crank–Nicolson method experiences difficulty with increasing k. With $v = 5$, the Crank–Nicolson method also loses accuracy with increasing k while it is preserved with all nine SLMMs.

Table 6. Maximum error

Method	t	$k = 1$	$k = 2$	$k = 3$	$k = 5$	$k = 10$
CN	1.0	0.18E − 4	0.88E − 5	0.88E − 5	0.10E − 2	0.14E − 0
	2.0	0.17E − 8	0.83E − 9	0.83E − 9	0.10E − 5	0.18E − 1
SM12	1.0	0.82E − 5	0.41E − 5	0.41E − 5	0.41E − 5	0.41E − 5
	2.0	0.82E − 9	0.41E − 9	0.41E − 9	0.41E − 9	0.41E − 9
SM12E	1.0	0.78E − 5	0.39E − 5	0.39E − 5	0.39E − 5	0.39E − 5
	2.0	0.78E − 9	0.39E − 9	0.39E − 5	0.39E − 5	0.39E − 5
SM22	1.0	0.89E − 4	0.44E − 4	0.44E − 4	0.44E − 4	0.44E − 4
	2.0	0.53E − 8	0.26E − 8	0.26E − 8	0.26E − 8	0.26E − 8
SM23	1.0	0.49E − 5	0.24E − 5	0.24E − 5	0.24E − 5	0.24E − 5
	2.0	0.53E − 9	0.27E − 9	0.27E − 9	0.27E − 9	0.27E − 9
SM23E	1.0	0.27E − 4	0.13E − 4	0.13E − 4	0.13E − 4	0.13E − 4
	2.0	0.25E − 8	0.12E − 8	0.12E − 8	0.12E − 8	0.12E − 8
SM33	1.0	0.34E − 4	0.17E − 4	0.17E − 4	0.17E − 4	0.17E − 4
	2.0	0.44E − 8	0.22E − 9	0.22E − 9	0.22E − 9	0.22E − 9
SM34	1.0	0.90E − 6	0.45E − 6	0.10E − 4	0.53E − 5	0.45E − 6
	2.0	0.99E − 10	0.49E − 10	0.49E − 10	0.49E − 10	0.49E − 10
SM34E	1.0	0.94E − 6	0.47E − 6	0.40E − 5	0.11E − 8	0.47E − 6
	2.0	0.10E − 9	0.52E − 10	0.32E − 9	0.58E − 10	0.52E − 10
SM44	1.0	0.14E − 4	0.74E − 5	0.70E − 5	0.69E − 5	0.69E − 5
	2.0	0.15E − 8	0.75E − 9	0.75E − 9	0.75E − 9	0.75E − 9

REFERENCES

1. J. R. Cash, Two new finite difference schemes for parabolic equations. *SIAM Jl numer. Analysis* **21**, 433–446 (1984).
2. A. R. Gourlay and J. Ll. Morris, The extrapolation of first order methods for parabolic partial differential equations. II. *SIAM Jl numer. Analysis* **17**, 641–655 (1980).
3. A. R. Gourlay and J. Ll. Morris, Linear combinations of generalised Crank–Nicolson schemes. *IMA Jl numer. Analysis* **1**, 347–357 (1981).
4. J. C. Butcher, Coefficients for the study of Runge–Kutta integration processes. *J. Aust. math. Soc.* **3**, 185–201 (1963).
5. J. R. Cash, The integration of stiff initial value problems in odes using modified extended backward differentiation formulae. *Comput. Math. Applic.* **9**, 645–657 (1983).
6. J. R. Cash, On the integration of stiff systems of O.D.E.'s using extended backward differentiation formulae. *Num. Math.* **34**, 235–246 (1980).
7. J. R. Cash, Split linear multistep methods for the integration of stiff differential systems. *Num. Math.* **42**, 299–310 (1983).
8. W. Liniger and R. A. Willoughby, Efficient numerical integration methods for stiff systems of differential equations. IBM Res. Rep. RC-1970 (1967).
9. J. D. Lambert, *Computational Methods in Ordinary Differential Equations*. Wiley, New York (1973).
10. J. Schur, Über Potenzreihen die im Innern des Einheitskreises beschrankt sind. *J. reine angew. Math.* **147**, 205–232 (1916).